201-16128

HIGH PRODUCTION VOLUME (HPV)

CHEMICALS CHALLENGE PROGRAM

TEST PLAN

For

3-Cyclohexene-1-carboxylic acid, 3-cyclohexen-1-ylmethyl ester (Diene 221)

CAS NO. 2611-00-9

December 2005

Prepared by:

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EXECUTE SUMMARY

The Dow Chemical Company voluntarily submits the following screening information data and Test Plan covering the chemical 3-cyclohexene-1-carboxylic acid, 3-cyclohexen-1-ylmethyl ester, also known as Diene 221 (CAS No. 2611-00-9), for review under the Environmental Protection Agency's High Production Volume (HPV) Chemicals Challenge Program. Since this material is produced in a closed system at one site and as an intermediate is rapidly reacted to produce the final product, a limited amount of physical chemical and mammalian toxicity data exists to evaluate the potential hazards associated with Diene 221. Two moles of tetrahydrobenzaldehyde (THBA) are reacted to produce a mole of Diene 221. Peracetic acid is subsequently reacted with Diene 221 to produce the final product. Available data for the Diene 221 precursor, THBA, which is expected to be metabolized to the same degradation product as Diene 221, tetrahydrobenzoic acid, is presented. Thus, the information on THBA is expected to serve as a surrogate for Diene 221. Both THBA and peracetic acid are corrosive materials. Since Diene 221 is a closed system intermediate there is no need for a reproduction study. Based on the limited number of workers exposed to this material, the corrosive nature of THBA and peracetic acid which have resulted in a high degree of personal protective equipment whenever exposure is possible, the available data on THBA is considered sufficient to address the biodegradation and environmental and mammalian toxicology HPV endpoints. However, the HPV physical chemical endpoints will be measured and the fugacity models recalculated.

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TEST PLAN FOR
3-Cyclohexene-1-carboxylic acid, 3-cyclohexen-1-ylmethyl ester (Diene 221)

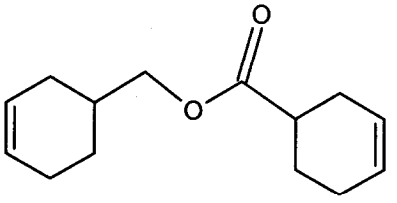
CAS Nos. 2611-00-9

I. INTRODUCTION AND IDENTIFICATION OF CHEMICAL

Under EPA's High Production Volume (HPV) Chemicals Challenge Program, The Dow Chemical Company (Dow) has committed to voluntarily compile basic screening data on 3-cyclohexene-1-carboxylic acid, 3-cyclohexen-1-ylmethyl ester (Diene 221). The data included in this Test Plan include physicochemical properties, environmental fate, and human and environmental effects of Diene 221, as defined by the Organization for Economic Cooperation and Development (OECD). Because Diene 221 is an ester, esterases as well as alcohol and aldehyde dehydrogenases present in microorganisms, aquatic species and mammals should rapidly degrade Diene 221 and tetrahydrobenzaldehyde (THBA) to the same degradation product. Thus information on THBA, also part of the EPA's HPV program, is also provided. The information provided comes from existing data developed by or on behalf of Dow, or is found in the published scientific literature.

A. Structure and Nomenclature

Following is a structural characterization of Diene 221 and its associated nomenclature.



Diene 221

B. Manufacturing & Use

Union Carbide Corporation, a subsidiary of The Dow Chemical Company, operates a single manufacturing site producing Diene 221. Two moles of THBA are reacted to produce a mole of Diene 221 which is subsequently reacted with peracetic acid to produce the final product.

THBA has an odor threshold of approximately 0.22 ppm, and will be detected by smell before air concentrations reach unsafe levels.

Approximately 50 individuals are involved in the manufacture or use of THBA and these individuals have extremely low potential for skin and airborne exposure. Due to the subacute hazards associated with exposure to THBA, an occupational exposure limit of 5 ppm (Union Carbide Occupational Exposure Guideline) has been set. This has resulted in specific manufacturing procedures and practices to minimize the exposure potential to THBA. Between 1988 and 1998, over 300 samples were obtained

from the THBA production and use plants. Only two values were greater than 1 ppm, and both of these were below the UCC Occupational Exposure Guideline. A review of more recent industrial hygiene samples from 1999 to the present in both manufacturing and use facilities have also shown that all samples are 1 ppm or lower. Due to the corrosive nature of THBA, personal protective equipment including (self-contained breathing apparatus (SCBA) when vapor exposure is high (considered to be greater than the action level (2.5 ppm) of the UCC Occupational Exposure Guideline), monogoggles, gloves and chemical apron, are worn whenever exposure to THBA is possible. Such operations could include sampling and material transfer operations, shutdown and clean-up activities.

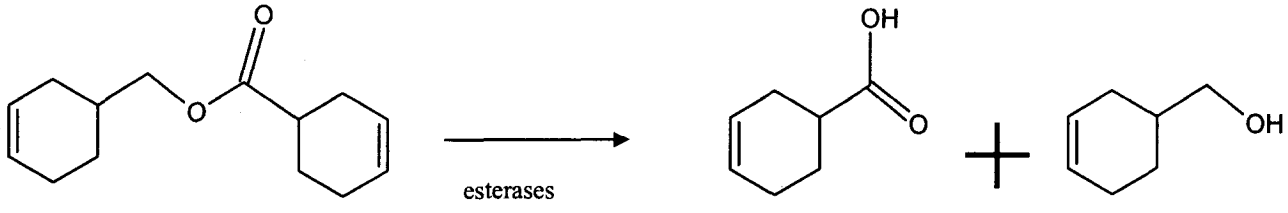
Following the production of Diene 221, the material undergoes another chemical reaction with peracetic acid to produce the final product. Roughly the same number of individuals work in this plant as in the THBA plant. The amount of Diene 221 present in the final product is expected to be very low, probably less than 1 ppm.

Peracetic acid, C_2O_3, has an odor threshold estimated to be 50 ppb (Ancker and Zetterberg, 1997). Peracetic acid has a pungent, vinegar-like odor (Swern, 1970). Concentrations of 150 ppb are considered tolerable and not unpleasant to humans while 350 ppb are considered unpleasant when inhaled for long time periods (McDonagh, 1997). Typical concentrations of peracetic acid measured outside of the reactor are below the detection limit of 20 ppb. During maintenance, concentrations of <1 ppm peracetic acid have been measured. Since peracetic acid is corrosive to the skin and eyes, protective equipment required during maintenance includes full-face respirator, air-purifying or positive-pressure supplied-air respirator, and full chemical resistant suit depending on operation.

Due to the corrosive nature of both THBA and peracetic acid, the personal protective equipment worn to prevent exposure to either of these chemicals will also protect workers from exposure to Diene 221. Since Diene 221 is less volatile than either THBA or peracetic acid, exposure to Diene 221 should be well below the measured values for THBA or peracetic acid. Since Diene 221 is produced and reacted in a closed system, release to the environment is expected to be quite rare.

II. METABOLISM.

Uptake of Diene 221 by microorganisms, aquatic species or mammals is expected to result in quite rapid metabolism by esterases resulting in formation of tetrahydrobenzoic acid and tetrahydrobenzyl alcohol. The tetrahydrobenzyl alcohol is expected to be rapidly metabolized to the aldehyde, tetrahydrobenzaldehyde (THBA), the precursor for Diene 221. THBA will be rapidly metabolized to the acid. The two enzymes forming the aldehyde and the acid are alcohol dehydrogenase and aldehyde dehydrogenase. These reactions are expected to occur relatively rapidly. Therefore available toxicity data for THBA should be relevant and acceptable for Diene 221 and tetrahydrobenzoic acid.

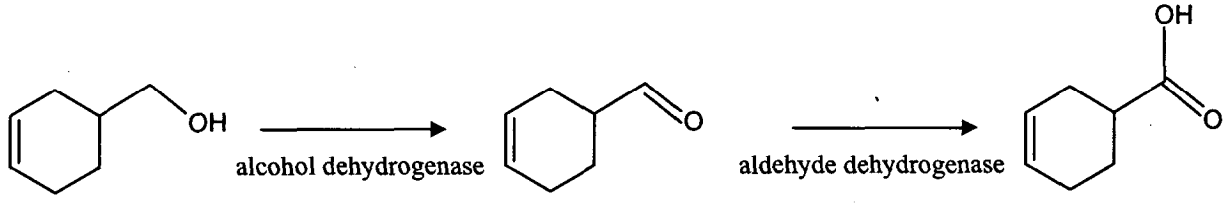


Diene 221
Tetrahydrobenzyl

Tetrahydrobenzoic

Acid

Alcohol



Tetrahydrobenzyl
Alcohol

Tetrahydrobenzaldehyde

Tetrahydrobenzoic
Acid

III. TEST PLAN RATIONALE

The information included in this Test Plan has come from one or more of the following sources:
1) Internal studies conducted by or on behalf of The Dow Chemical Company
2) Studies that have been extracted from the scientific literature either as primary references, or as reported in well-accepted, peer-reviewed reference books
3) Calculation methods or quantitative structure-activity relationships (QSAR) which are accepted by the US EPA for such purposes (1999b).

This assessment includes information on physicochemical properties, environmental fate, and human and environmental effects associated with Diene 221. Information is also provided for THBA since Diene 221 is expected to be metabolized to tetrahydrobenzoic acid in either aquatic or mammalian organisms. The data used to support this program include those Endpoints identified by the US EPA (1998). Key studies have been identified for each data Endpoint, and are summarized in Robust Summary form in Section VII of this Dossier.

All studies were reviewed and assessed for reliability according to standards specified by Klimisch *et al* (1997), as recommended by the US EPA (1999a). The following criteria were used for codification:
1. Valid without Restriction - Includes studies which comply with US EPA and/or OECD-accepted testing guidelines, which were conducted using Good Laboratory Practices (GLPs) and for which test parameters are complete and well documented,
2. Valid with Restrictions – Includes studies which were conducted according to national/international testing guidance and are well documented. May include studies conducted prior to establishment of testing standards or GLPs but meet the test parameters and data documentation of subsequent guidance;

also includes studies with test parameters which are well documented and scientifically valid but vary slightly from current testing guidance. Also included are physical-chemical property data obtained from reference handbooks as well as environmental endpoint values obtained from an accepted method of estimation (i.e. EPIWIN).
3. Not Valid – Includes studies in which there are interferences in either the study design or results that provide scientific uncertainty or where documentation is insufficient.
4. Not Assignable – Includes studies in which limited data is provided.

Those studies receiving a Klimisch rating of 1 or 2 are considered adequate to support data assessment needs in this Test Plan.

IV. TEST PLAN SUMMARY AND CONCLUSIONS

Physical-chemical property values (Melting Point, Boiling Point, Vapor Pressure, Partition Coefficient and Water Solubility) were calculated. We know the melting point is lower than the estimated value of 46.9°C since it is a liquid at room temperature, 25°C. Therefore, we will repeat the physical property measurements as regards melting point, boiling point, vapor pressure, water solubility and Kow. The partition coefficient, log Kow, is approximately 5. Although the log Kow is estimated to be nearly 5, the activity of esterases upon Diene 221 will increase the water solubility of the resultant products.

Environmental Fate values for Hydrolysis, Photodegradation, and Transport (Fugacity) were obtained using computer estimation –modeling programs. The model predicts Diene 221 will slowly hydrolyze. The fugacity model level 3 predicts that most of the material emitted will end up in soil (65%) with 15.6% in water and 19% in sediment. A very small amount will remain in air. Any material that is released to the air will be rapidly photodegraded via reaction with hydroxyl radical and ozone. The AopWin predicted half life in the atmosphere is approximately 41 minutes (0.7 hr.). Four of the 6 biodegradation computer estimation-modeling programs (Biowin (v4.02) predict the material will biodegrade rapidly. The primary biodegradation timeframe is predicted to be days while the ultimate biodegradation timeframe is weeks. Thus all of the models predict Diene 221 will degrade quite rapidly. Esterases are expected to degrade Diene 221 to the acid and the alcohol. The alcohol will be rapidly degraded to the aldehyde and then to the acid. The aldehyde, THBA, was shown to be readily biodegradable, using a test procedure which was equivalent to OECD Test Guideline 301D. Thus models and available data on structurally similar material indicate Diene 221 will be degraded very rapidly.

Ecotoxicity values for Diene 221 have been estimated for fish, daphnia and algae. The estimated values range from 0.08 mg/L in algae to 0.86 mg/L in fish. Since aquatic organisms have esterase enzymes Diene 221 should be rapidly metabolized to tetrahydrobenzoic acid and tetrahydrobenzyl alcohol. The alcohol should be further metabolized to the aldehyde and then to the acid. Thus the available data for THBA should be representative for Diene 221 also and would predict much higher LC50 and EC50 values than has been estimated for Diene 221.

Mammalian Toxicity endpoints are limited to acute parameters. The material causes minor irritation in dermal and eye irritation studies. The dermal LD50 value is $\geq$12325 mg/kg while the oral LD50 ranges from 1363 mg/kg in females to 2386 mg/kg in males. The lowest oral LD50 value is approximately half that of THBA which supports the premise that Diene 221 and THBA are rapidly metabolized to common degradation products.

Although no repeated dose, mutagenicity or developmental toxicity data is available, several two week studies have been conducted on THBA via two different routes. As part of these studies, the testes and ovaries were weighed and testes examined histopathologically. However, for reproductive toxicity purposes, these studies were of short duration and therefore rated a 4 in the Klimisch rating system. Although the study was of a short duration, there were no significant treatment-related effects noted which would indicate a reproductive effect. No developmental toxicity study was found. Point mutation and chromosomal aberration assays of THBA were negative. Given that Diene 221 and THBA are expected to be metabolized to common degradation products and given that Diene 221 is used as a closed system intermediate and exposure will be limited due to the corrosive nature of other chemicals used in it's manufacture, additional toxicity studies are considered unnecessary.

A tabular depiction of data availability and testing recommendations for Diene 221 can be found in Table 1.

V. DATA SET SUMMARY AND EVALUATION

The key studies used in this assessment to fulfill the HPV requirements have been placed in an Endpoint-specific matrix, and are further discussed below. Robust Summaries for each study referenced can be found in Section VII of this dossier.

A. Chemical/Physical Properties

All HPV Endpoints for Chemical/Physical Properties have been calculated for Diene 221 (Table 2). Additional information is provided from the THBA test plan. The melting point is estimated to be 47°C, indicating Diene 221 is a solid at room temperature. However, the material is a liquid at room temperature. We will repeat the physical property measurements as regards melting point, boiling point, vapor pressure, water solubility and Kow.

B. Environmental Fate and Biodegradation

All HPV Endpoints for Environmental Fate have been calculated for Diene 221 (Table 3). Additional information is provided from the THBA test plan. Based on the presence of esterases and alcohol and aldehyde dehydrogenases in microorganisms, Diene 221 and THBA are expected to be rapidly degraded to tetrahydrobenzoic acid. THBA has been reported to be readily biodegradable in an OECD 301D test. The Fugacity Model will be recalculated with actual physical chemical values.

C. Aquatic Toxicity

Aquatic toxicity data has been calculated for fish, daphnia and algae for Diene 221 (Table 4). Calculated acute ecotoxicity values were estimated using the esters class in the ECOSAR v0.99h program. Additional information is provided from the THBA test plan. Based on the presence of esterases and alcohol and aldehyde dehydrogenases in all aquatic genera used for toxicity testing, we would expect the LC50 or EC50 values to be approximately half the value for THBA. The Diene 221values are predicted to be half of the THBA value, since two moles of THBA are produced for each mole of Diene 221.

D. Mammalian Toxicity Endpoints

Summaries of available toxicity data used to fulfill the HPV Endpoints for Mammalian Toxicity are found in Tables 5-7. Each of the Key Studies has been further summarized in the Robust Summary section of this Dossier. Additional information is provided from the THBA test plan.

1.0 Acute Toxicity

The acute oral LD_{50} values are 1363 mg/kg and 2386 mg/kg in female and male rats, respectively. The acute dermal LD50 is $\geq$12,325 mg/kg. A saturated atmosphere did not produce lethality. Diene 221 produced minor erythema to the skin and minor conjunctival irritation. There was no evidence of corneal damage. Based on the presence of esterases and alcohol and aldehyde dehydrogenases in all mammals, Diene 221 and THBA are expected to be metabolized to common degradation products. There appears to be reasonably good agreement between the Diene 221 oral LD50 value for rats with that of THBA. Given that Diene 221 produces only minor irritation to the skin and the larger MW of this material, the dermal LD50 is much greater than for THBA which is a corrosive material.

2.0 Repeated Dose Toxicity

There is no repeated dose toxicity data for Diene 221. However, two separate two-week inhalation toxicity studies, as well as a two-week dermal toxicity study have been conducted with THBA (Table 6). Doses causing severe irritation at the application site in the dermal study produced only slight effects (mineral deposits) in the kidney. Inhalation exposure to THBA resulted in histopathologic changes in the nasal tissues. In these same animals, clinical changes in kidney function were observed, which included decreases in urine volume, pH and osmolality. However, there was no evidence of histopathologic changes. Thus, following the two most likely routes of exposure for humans, only minimal changes were observed at levels which resulted in severe irritation at the portal of entry.

3.0 Developmental Toxicity

There is no available developmental toxicity study (Table 6). However due to the corrosive nature of the precursors used to manufacture Diene 221 or subsequently reacted with Diene 221 an increased level of personal protective equipment is required. Given the limited number of individuals exposed to Diene 221 and the low concentrations of THBA or peracetic acid measured in the workplace, a developmental toxicity study of Diene 221 is considered to be unnecessary.

4.0 Reproductive Toxicity

There is no available reproduction toxicity study (Table 6). Several two week studies have been conducted via two different routes of THBA. As part of these studies, the testes and ovaries were weighed and testes examined histopathologically. However, for reproductive toxicity purposes, these studies were of short duration and therefore rated a 4 in the Klimisch rating system. Although the study was of a short duration and produced severe irritation at the dermal application site and slight effects in the kidney, there were no significant treatment-related effects noted which would indicate a reproductive effect. Since the material is used solely as a chemical intermediate with limited worker exposure, a reproductive toxicity study is considered unnecessary.

5.0 Mutagenicity and Chromosomal Aberrations

5.1 Mutagenicity Testing (Ames test)
There is no available data on Diene 221. THBA was negative in the Ames test.

5.2 - Chromosomal Aberrations
There is no available data on Diene 221. THBA was negative in the in vitro CHO/HGPRT assay and in the in vivo mouse micronucleus assay.

If we are unable to document the physical chemical properties cited on the MSDS, the following physical chemical measurements will be conducted: melting point, boiling point, vapor pressure, water solubility and Kow. The Fugacity Model will be recalculated with actual physical chemical values. Although there is no toxicity data for Diene 221, it is expected to rapidly be degraded by esterases and alcohol and aldehyde dehydrogenases to tetrahydrobenzoic acid. Since it is a closed system intermediate with a minimal number of individuals who are required to wear protective gear to reduce exposure to other chemicals in the workplace, no additional toxicity studies are necessary.

VI. REFERENCES

ACGIH TLV (2002). Threshold Limit Values for chemical substances and physical agents and Biological Exposure Indices. American Conference of Governmental Industrial Hygienists.

Ancker, K. and Zetterberg, L. (1997). Measurement of peracetic acid at Eka Chemicals AB, Bohus. Unpublished report A97329 for Eka Chemicals. Cited in ECETOC (2001). Peracetic acid (Cas No. 79-21-0) and its equilibrium solutions. JACC # 40.

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Swern, D. (1970). Organic peroxides Vol 1. Wiley Interscience, New York, NY, USA, pp340-369, 461-474 Cited in ECETOC (2001). Peracetic acid (Cas No. 79-21-0) and its equilibrium solutions. JACC # 40.

US EPA, (1998). Guidance for meeting the SIDS requirements (The SIDS Guide). Guidance for the HPV Challenge Program (11/31/98).

US EPA, (1999a). Determining the adequacy of existing data. Guidance for the HPV Challenge Program (2/10/99).

US EPA, (1999b). The use of structure-activity relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA.

VI. ROBUST STUDY SUMMARIES -IUCLID

Data Sets are appended

Table 1. Test Plan Matrix for Diene 221

	Info available?	OECD?	GLP?	Other study based on THBA	Estimated method?	Acceptable?	Testing recommendation?
PHYSICAL CHEMICAL							
Melting Point	Y	N	N	N	Y	Y, 2	Y
Boiling Point	Y	N	N	N	Y	Y, 2	Y
Vapor Pressure	Y	N	N	N	Y	Y, 2	Y
Partition Coefficent	Y	N	N	N	Y	Y, 2	Y
Water Solubility	Y	N	N	N	Y	Y, 2	Y
ENVIRONMENTAL FATE ENDPOINTS							
Photodegradation	Y	N	N	N	Y	Y, 2	N
Biodegradation	Y	N	N	Y	Y	Y, 2	N
Hydrolysis	Y	N	N	N	Y	Y, 2	N
Transport between Environmental Compartmenats (Fugacity)	Y	N	N	N	Y	Y, 2	Y
Bioaccumulation	N	N	N	N	N	N	N
ECOTOXICITY							
Acute Toxicity to Fish	Y	N	N	Y	Y	Y, 2	N
Acute Toxicity to Aquatic Invertebrates	Y	N	N	Y	Y	Y, 2	N
Acute Toxicity to Aquatic Plants	Y	N	N	N	Y	Y, 2	N
MAMMALIAN TOXICITY							
Acute Toxicity	Y	Y	Y	Y	N	Y, 1A	N
Repeated Dose Toxicity	Y	N	N	Y	N	Y, 2	N
Genetic Toxicity - Mutation (Ames)	Y	N	N	Y	N	Y, 2	N
Genetic Toxicity - Chromosomal Aberrations	Y	N	N	Y	N	Y, 2	N
Developmental Toxicity	N	N	N	N	N	N	N
Reproductive Toxicity	N	N	N	N	N	N	N

Y = Yes; N = No; ND = No Data; S = Supplemental, not required under HPV; - = Not applicable

Table 2. Matrix of Available and Adequate Data on Diene 221
Physicochemical Properties

Name (CAS No.)	Melting Point (°C)	Vapor Pressure (hPa @ 25°C)	Boiling Point (°C)	Partition Coefficient (log Kow)	Water Solubility (mg/L @ 20C)
Diene 221 (2611-00-9)	46.9 (calculated)	0.00175 (calculated)	299 (calculated)	4.97 (calculated)	1.94 (calculated)
TETRAHYDROBENZALDEHYDE (THBA) (100-50-5)	-96.1 (measured)	2.97 (2.225 mm Hg) (calculated)	164 (measured)	1.89 (preferred calc.) 1.34 (other calc.)	0.5% Slightly soluble (measured)

Table 3. Matrix of Available and Adequate Data on Diene 221
Environmental Fate

Name (CAS No.)	**Hydrolysis**	**Photodegradation** Half life	**Biodegradation**	**Environmental Transport** Level III 1000 kg/hr released to air, water and soil
Diene 221 (2611-00-9)	Half life 9.2 years at 25C and pH 7 (calculated)	Hydroxyl Radicals Reaction: 126.5794 E-12 Ozone Reaction: 40.000000 E-17 cm3/molecule-sec Overall half life = 41 minutes (calculated)	Predicted to biodegrade rapidly (calculated)	Air 0.1% Water 15.6% Soil 65.3% Sediment 19%
Tetrahydrobenzadehyde (THBA) (100-50-5)	Not estimatable (Hyrowin 1.67) Does not contain hydrolyzable groups	Hydroxyl Radicals Reaction: 88.6330 E-12 Ozone Reaction: 20.000000 E-17 cm3/molecule-sec Overall half life = 0.7 hours (~42 minutes) (calculated)	readily biodegradable 76% in a closed bottle test equivalent to OECD 301D	Air 0.035% Water 99.9% Soil 0.0033% Sediment 0.074%

Table 4. Matrix of Available and Adequate Data on Diene 221
Ecotoxicity

Name (CAS No.)	Acute Fish 96-hour LC50 (mg/l)	Acute Invertebrate 48-hour EC50 (mg/l)	Algal 72-hour growth inhibition EC50 (mg/l)
Diene 221 (2611-00-9)	~0.859 (estimated)	~0.347 (estimated)	~0.076 (estimated)
Tetrahydrobenzadehyde (THBA) (100-50-5)	No data for acute study Predicted 96 hr LC50 9.997 mg/L Chronic 14-day LC50 is 1.1 mg/L Predicted 32-day Chronic Value (ChV) is 0.885 mg/L	130 Predicted 48 hr LC50 6.85 mg/L	No data for acute study Predicted 96 hr EC50 68.4 mg/L

Table 5. Matrix of Available and Adequate Data on Diene 221
Acute Toxicity

Name (CAS No.)	Acute Oral	Acute Inhalation	Acute Dermal	Dermal Irritation	Eye Irritation	Sensitization
Diene 221 (2611-00-9)	1363 mg/kg females 2386 mg/kg males (measured)	> saturated atmosphere	≥12,325 mg/kg	Minor erythema	Minor conjunctival irritation	No Data
Tetrahydrobenzadehyde (THBA) (100-50-5)	2385 mg/kg	>1679 ppm for 6 hour exposure	1716mg/kg	Corrosive according to DOT test	Moderately severe corneal injury using 0.005 ml test material	No data

Table 6. Matrix of Available and Adequate Data on Diene 221
Repeat-dose Toxicity

Name (CAS No.)	Repeat Dose	Reproductive	Developmental
Diene 221 (2611-00-9)	No Data	No Data	No Data
Tetrahydrobenzadehyde (THBA) (100-50-5)	Two week inhalation NOEL – 5 ppm Two week dermal systemic NOEL – 0.10 ml/kg/day	No effect on ovary or testicular weights or testes histopath in two week dermal study	No data

Table 7. Matrix of Available and Adequate Data on Diene 221
Genotoxicity

Name (CAS No.)	Genotoxicity (*in vitro* -bacterial)	Genotoxicity (*in vitro* - mammalian)	Genotoxicity (*in vivo*)
Diene 221 (2611-00-9)	No Data	No Data	No Data
Tetrahydrobenzadehyde (THBA) (100-50-5)	Negative	Negative in CHO/HGPRT assay	Negative in mouse micronucleus assay

Table 8
Test Plan Matrix for Diene 221

	Diene 221 (2611-00-9)	Tetrahydrobenzaldehyde (THBA) (100-50-5)
Melting point, °C	-66 A	-96.1 (measured) A
Boiling point, °C	276 A	164 (measured) A
Vapor Pressure, hPa at 25°C	0.00175 (calculated) A	2.97 (calculated) A
Water Solubility , mg/L @20°C	1.94 (calculated) A	0.5% (measured) Slightly soluble A
K_{ow}	4.97 (calculated) A	1.89(calculated) A
Biodegradation	Predicted to readily degrade A	76% in closed bottle test equivalent to OECD 301D readily biodegradable A
Hydrolysis, half life at 20°C and pH 7	Does not contain hydrolysable groups A	Does not contain hydrolysable groups A
Photodegradability	Overall half life = 41 minutes A	Overall half life = 0.7 hours A
Transport between Environmental Compartments: **(Fugacity Level III Model)** Default assumption: 1000 kg/hr released into air, water, and soil.	Air 0.1% Water 15.6% Soil 65.3% Sediment 19% A	Air 0.035% Water 99.9% Soil 0.0033% Sediment 0.074% A
Acute Toxicity to Fish (96hr LC50)	~0.859mg/L (calculated) A	14-day is 1.1 mg/L (measured) A
Acute Toxicity to Aquatic Invertebrates (48hr EC50)	~0.347 mg/L (calculated) A	130 (measured) A
Toxicity to Aquatic Plants (72hr EC50)	~0.076 mg/L (calculated) A	68.4 (calculated)
Acute Toxicity (oral), mg/kg	≥1363 mg/kg A	2385 mg/kg A
Acute Toxicity (dermal) ml/kg	≥12,325 mg/kg	1716 mg/kg A
Acute Eye Irritation	Minor conjunctival irritation	Moderately severe corneal injury

	A	using 0.005 ml test material A
Acute Skin Irritation	Minor erythema A	Corrosive according to DOT test A
Repeated Dose Toxicity	No data R	Two week NOEL – 5 ppm A
Genetic Toxicity-Mutation	No data R	Negative A
Genetic Toxicity- Chromosomal Aberrations	No data R	Negative (in vitro) Negative (in vivo) A
Toxicity to Reproduction	No data NR	No data NR
Developmental Toxicity	No data NA	No data NA

Legend	
Symbol	**Description**
R	Endpoint requirement fulfilled using category approach, SAR
Test	Endpoint requirements to be fulfilled with testing
Calc	Endpoint requirement fulfilled based on calculated data
A	Endpoint requirement fulfilled with adequate existing data
NR	Not required per the OECD SIDS guidance
NA	Not applicable due to physical/chemical properties